

CLAIMS

1. A method of investigating different physical and/or chemical forms of a material, the method comprising:

5

providing an array of receptacles each containing material (hereinafter "said initial material") to be investigated;

10 subjecting said initial material in respective different receptacles to respective different treatments under the control of a computer; and

15 analysing any material resulting from said different treatments (hereinafter "said resultant material").

2. A method according to Claim 1 which includes associating data relating to the analysis of each resultant material with information relating to the 20 treatment(s) used to prepare said resultant material from said initial material.

3. A method according to Claim 1 or Claim 2, wherein data relating to said analysis is stored in said computer and 25 associated with said information relating to the treatment.

4. A method according to any preceding claim, wherein said computer is programmed to determine treatments to 30 which initial material in receptacles is to be subjected.

5. A method according to Claim 4, wherein said computer determines treatments in dependence upon the results of

the analysis of resultant material in a first series of experiments using said array.

6. A method according to any preceding claim, wherein
5 said initial material is a solid.

7. A method according to any preceding claim, wherein
said different treatments to which initial material is
subjected to prepare resultant material includes
10 variable(s) relating to the solvent or solvents used in
the treatments (hereinafter referred to as "solvent
variables").

8. A method according to Claim 7, wherein said solvent
15 variables are selected from one or more of the following:

a first solvent variable relating to the number of
solvents used for preparing resultant material from
initial material;

20 a second solvent variable relating to the timing of the
addition of the solvent or solvents into a receptacle;

a third solvent variable relating to the amount of a
25 solvent or solvents used in a treatment; and

a fourth solvent variable relating to the identity of a
solvent or solvents used.

30 9. A method according to Claim 8, wherein at least two of
said solvent variables are varied in a single series of
experiments using said array and/or in multiple series of
experiments.

10. A method according to Claim 8 or Claim 9, wherein the implementation of said solvent variables is under the control of said computer.

5

11. A method according to any preceding claim, wherein said different treatments to which initial material is subjected to prepare resultant material include a variable relating to the duration of the treatment of said initial 10 material to prepare said resultant material (hereinafter "said duration variable").

12. A method according to any preceding claim, wherein said different treatments to which initial material is subjected to prepare resultant material include a variable relating to the operation of a heating means during the treatments (hereinafter referred to as "heating 15 variables").

20 13. A method according to Claim 12, wherein said heating variables are selected from one or more of the following:

a first heating variable relating to the time of operation of said heating means;

25

a second heating variable relating to the duration of operation of said heating means; and

30 a third heating variable relating to whether operation of said heating means is continuous or in stages.

14. A method according to any preceding claim, wherein said different treatments to which initial material is

subjected to prepare resultant material include a variable relating to the operation of a cooling means during the treatments (hereinafter referred to as "cooling variables").

5

15. A method according to any preceding claim, wherein said different treatments to which initial material is subjected to prepare resultant material include variables relating to the agitation of material in the receptacles 10 during treatment (hereinafter referred to as "agitation variables").

16. A method according to Claim 15, wherein said agitation variables are selected from one or more of the following:

15

a first agitation variable relating to the time of operation of an agitation means for agitating material;

20 a second agitation variable relating to the duration of operation of said agitation means;

a third agitation variable relating to whether operation of said agitation means is continuous or in stages; and

25 a fourth agitation variable relating to the rate of operation of said agitation means.

17. A method according to any preceding claim, wherein a temperature profile is defined for each receptacle in the 30 array and data relating to the temperature profile is stored in said computer.

18. A method according to any preceding claim, which includes supporting said initial material on a porous member which is porous to fluids but not to said initial material.

5

19. A method according to any preceding claim, which includes applying a pressure to prevent solvent(s) passing out of the receptacles, away from said initial material, during treatment of the initial material.

10

20. A method according to Claim 19, wherein application of said pressure is controlled by said computer.

15

21. A method according to any preceding claim, wherein said resultant material is analysed and/or liquid removed from the receptacles is analysed.

22. A method according to any preceding claim, wherein said method is for:

20

investigating polymorphs of a material;

investigating isomers of a material in a manner which allows different isomeric forms to be resolved;

25

investigating different hydrates/solvates of a material;
or

investigating different salts of a material.

30

23. A method according to any preceding claim which comprises investigating polymorphs of said initial material and the method including the step of providing

initial material in the receptacles and subjecting said material to different treatments, wherein treatments between receptacles in the array vary in terms of one or more of said solvent variables as described in Claim 8; 5 and/or duration variables as described in Claim 11; and/or heating variables as described in Claim 12; and/or cooling variables as described in Claim 14; and/or agitation variables as described in Claim 16; and/or by having different temperature profiles as described in Claim 17; 10 and, at the end of a treatment in a first series of experiments using said array, analysing resultant materials if produced to determine if different polymorphs have been prepared.

15 24. A method according to Claim 23, the method including a further step of using said computer to determine variables to be adopted in a second series of experiments using said array with a view to locating additional polymorph(s).

20 25. A method according to any of claims 1 to 22, wherein the method is for the resolution of isomers of said initial material and includes the steps of:

25 treating the initial material with a range of potential salt forming materials (hereinafter "salt formers") with a view to preparing salts of said initial materials; subjecting the materials in said receptacles to different treatments; and, after such treatments, analysing the resultant material or liquid removed from said 30 receptacles.

26. A method according to any of claims 1 to 22, the method being for investigating different salts of a

material and comprising the steps of treating the initial material with a range of potential salt forming materials (hereinafter "salt formers") and subjecting the materials to different treatments with a view to re-crystallising 5 the salts of the initial material; and, thereafter, analysing the resultant materials.

27. A method of examining the effects in a treatment of a material of varying selected treatment variables, the 10 method comprising preparing a first resultant material from an initial material using a first treatment using a first set of experimental variables and preparing a second resultant material from an initial material using a second treatment using a second set of experimental variables, 15 wherein said first and second treatments are controlled by a computer.

28. A method of preparing a library of resultant materials using an array of receptacles each of which includes an 20 initial material, the method comprising varying selected treatment variables used to prepare resultant materials from said initial material, wherein the treatments to which said initial material are subjected are controlled by a computer.

25

29. A method of effecting automatically the preparation of resultant materials from initial material, the method comprising preparing resultant materials from initial material using respective sets of physical and/or chemical 30 treatments, wherein data relating to said sets is stored by a computer, and the treatments are undertaken under the control of the computer.

30. Apparatus for investigating different physical and/or chemical forms of a material, the apparatus comprising:

an array of receptacles for containing material
5 (hereinafter "initial material") to be investigated;

treatment means for subjecting initial material to respective different treatments; and

10 a computer arranged to control the respective different treatments to which initial material is subjected.

31. Apparatus according to Claim 30, wherein said receptacles include a porous member which is porous to fluids but not to said initial material, wherein said porous member defines a wall for supporting initial material.

32. Apparatus according to Claim 31, which includes pressure means for applying a pressure to restrict the passage of fluid from the receptacles under gravity.

33. Apparatus according to Claim 32, wherein said pressure means is controlled by said computer.

25

34. Apparatus according to any of Claims 30 to 33, wherein said treatment means includes temperature control means for varying the temperature of materials contained in said receptacles.

30

35. Apparatus according to Claim 34, wherein said temperature control means includes a heating means and/or

a cooling means controlled by said computer in a predetermined manner.

36. Apparatus according to any of Claims 30 to 35, wherein
5 means for condensing vapour is associated with said
receptacles for reducing loss of material therefrom by
evaporation.

37. Apparatus according to any of Claims 30 to 36, wherein
10 said treatment means includes agitation means for
agitating material in said receptacles.

38. Apparatus according to any of Claims 30 to 37, wherein
respective collection means are associated with each
15 receptacle in the array for collecting fluid passing out
of the receptacles.

39. Apparatus according to any of Claims 30 to 38, wherein
delivery means is provided for delivering materials into
20 the receptacles, said delivery means being arranged to
select materials from a material supply means and deliver
selected materials to a selected receptacle in a
predetermined amount and at a predetermined time.

25 40. Apparatus according to any of Claims 30 to 39, which
includes input means for inputting analytical data
relating to material produced after treatment of said
initial material into said computer, wherein said computer
is programmed to analyse data input into it and determine
30 variables to be used in a subsequent investigation on the
same initial material, using said apparatus.

41. The use of apparatus according to any of Claims 30 to 40 for investigating different physical and/or chemical forms of a material.
- 5 42. The use of apparatus according to any of Claims 30 to 40 in making a library of products.
- 10 43. The use of apparatus according to any of Claims 30 to 40 in effecting automatically a multiplicity of treatments of an initial material which treatments differ in at least one experimental variable.